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Random checkerboard based homogenization for estimating effective thermal conductivity of fully saturated soils

Dariusz Łydżba*, Adrian Różański, Magdalena Rajczakowska, Damian Stefaniuk

Department of Geotechnics, Hydrotechnics, Underground and Hydraulic Structures, Faculty of Civil Engineering, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, Wrocław, 50-370, Poland

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This paper proposes homogenization scheme for estimating the effective thermal conductivity of fully saturated soils. This approach is based on the random checkerboard-like microstructure. Two modeling scales and two modeling approaches are distinguished and used, i.e. microscale and mesoscale and 1-step and 2-step homogenizations, respectively. The 2-step homogenization involves sequential averaging procedure, i.e. first, at microscale, a mineralogical composition of soil skeleton is considered and averaging process results in estimation of the skeleton effective thermal conductivity, and then, at mesoscale, a random spatial packing of solid skeleton and pores via random checkerboard microstructure is modeled and leads to evaluation of the soil overall thermal conductivity. The 1-step homogenization starts directly at the mesoscale and homogenization procedure yields evaluation of the overall soil thermal conductivity. At the mesoscale, the distinct nature of soil skeleton, as composed of soil separates, is considered and random variability of soil is modeled via enriched random checkerboard-like structure. Both approaches, i.e. 1-step and 2-step homogenizations, interrelate mineralogical composition with the soil texture characterized by the volume fractions of soil separates, i.e. sand, silt and clay. The probability density functions (PDFs) of thermal conductivity are assumed for each of the separates. The soil texture PDF of thermal conductivity is derived taking into consideration the aforementioned functions. Whenever the random checkerboard-like structure is used in averaging process, the Monte Carlo procedure is applied for estimation of homogenized thermal conductivity. Finally, the proposed methodology is tested against the laboratory data from our measurements as well as those available from literature.

1. Introduction

Overall thermal conductivity of soil, λ^{hom}, is strongly dependent on soil mineral composition, texture, dry density, moisture content, porosity, etc. These properties can be easily evaluated from laboratory investigations, and therefore a large number of empirical/theoretical models for predicting thermal conductivity, based on the aforementioned characteristics, have been proposed in the literature (e.g. Mickley, 1951; Gemant, 1952; Woodside and Messmer, 1961; De Vries, 1963; Johansen, 1975; Campbell, 1985; Coté and Konrad, 2005; Lu et al., 2007, 2014). Furthermore, many attempts have been made in order to predict the thermal properties of soils using micromechanical models (e.g. Beran, 1968; Mori and Tanaka, 1973; Gruescu et al., 2007) or numerical calculations like those of finite element method (e.g. Kanit et al., 2003; El Moumen et al., 2015) or other methods.

Most of the methods for soil thermal conductivity prediction assume that the soil skeleton is a homogeneous medium characterized by the effective thermal conductivity λ_s. An appropriate estimation of skeleton conductivity λ_s is therefore a crucial point in formulation of an adequate predictor of the overall soil conductivity. A proper evaluation of skeleton conductivity would require a cumbersome and time-consuming laboratory investigation if it was realizable at all. In practice, the conductivity of soil skeleton is postulated ad hoc, without any scientifically based consideration, e.g. it is estimated using empirical formula as the function of clay (Gemant, 1952) or quartz (Johansen, 1975) content in the soil skeleton or, simply, each type of soil is assumed to be characterized by its own constant value of heat conductivity (e.g. Farouki, 1981).

* Corresponding author.
E-mail address: dariusz.lydzba@pwr.edu.pl (D. Łydżba).

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Considering the soil skeleton as a polycrystalline solid at the microscale and bearing in mind that various minerals are characterized by different values of thermal conductivity, the overall thermal conductivity of solid skeleton is mostly triggered by its mineral fabric. For instance, the thermal conductivity of quartz minerals is approximately a few times higher than that of clay. Furthermore, the thermal conductivities of an organic matter and other soil minerals differ by one order of magnitude. The additional difficulty arises from the fact that the same minerals can possess their own unique internal structure resulting in different values of thermal conductivity, e.g. thermal conductivity of quartz minerals might be in the range from 6 W m^{-1} K^{-1} to 11 W m^{-1} K^{-1} as reported by Clauser and Huenges (1995). Therefore, the proper mathematical description of heat conduction process, within the soil skeleton at the microscale, requires application of the random field theory and modeling the thermal conductivity as a random variable, with prescribed probability density function (PDF). Using the micromechanics approach, one can then evaluate, with presumed precision, the homogenized thermal conductivity of solid skeleton λ_s^{hom} in terms of mineral morphology of solid continuum under consideration. This value can then be used as the input parameter for the consideration at the mesoscale. At this scale, the soil is a medium composed, in general, of three phases, i.e. a solid skeleton with a three-dimensional (3D) structure of pore network filled with water and air. The aforementioned λ_s^{hom} can be treated as a material constant of a homogenized skeleton being the result of the smoothing procedure performed at the microscale. At the mesoscale, the spatial distribution of the thermal conductivity is associated with the spatial distribution of the phases composing the medium, i.e. solid, water and air. Here, on the contrary to the microscale, the components are characterized by three distinct values of thermal conductivity: λ_s^{hom} (skeleton), λ_{air} (air) and λ_w (water). Therefore, the randomness of the medium is only associated with the spatial distribution of the phases, while material constants are of deterministic type. Finally, the overall thermal conductivity λ^{hom} of soil can be, once again, evaluated using the micromechanics approach. The aforementioned method can be interpreted as a 2-step homogenization due to the number of scales involved in averaging procedure. This technique is theoretically justified only if a separation of scales exists, i.e. the size of the skeleton heterogeneities is significantly smaller than the average diameter of pores. The case of the soil skeleton composed of different soil separates with the sizes of the order of the average pore diameter does not exhibit a scale separation, at the mesoscale. The homogenization procedure can then be performed in one step by considering soil microstructure as composed of grains of soil separates characterized by own thermal conductivities and pores filled with water and air. The concept of effective thermal conductivity of soil skeleton cannot be used anymore in this case. Such methodology is called as a 1-step homogenization since mesoscale is only considered for averaging purpose.

In this paper, the considerations are limited to fully saturated soils. Therefore, the soil is treated as a two-phase medium with pores filled only with water. The overall thermal conductivity of soil-water mixture is evaluated by performing 2-step or 1-step homogenization, i.e. at the microscale and mesoscale or at the mesoscale only, respectively. Both analytical and computational micromechanics are performed for this purpose.

The paper is organized as follows. Section 2 provides basic principles and methods of micromechanics. The next section deals with the model development. Special attention is paid to formulation of analytical homogenization schemes for composite with components characterized by the random thermal conductivity coefficient with prescribed PDF. In addition, Hashin–Shtrikman (H–S)-like bounds are formulated. Using a 2-step homogenization methodology, three modeling scales are distinguished, i.e. the microscale, mesoscale and macroscale. At the microscale, the soil fabric is associated with textural class of the soil. The modeling consists in choosing an appropriate PDF of thermal conductivity and performing the homogenization scheme. As a result, the thermal conductivity of soil skeleton λ_s^{hom} is evaluated and then used as an input parameter at the mesoscale homogenization. At the mesoscale, the microstructure of the medium is considered as composed of homogenized solid skeleton and pores filled with water. The macroscale thermal conductivity λ^{hom}, called as the overall one, is estimated via Monte Carlo procedure, i.e. by performing a sequence of numerical simulations, for the checkerboard microstructure. The 1-step homogenization procedure is also used for evaluation of thermal conductivity of soil. This time the averaging procedure is performed using the enriched random checkerboard microstructure directly at the mesoscale. In Section 4, the verification of the proposed methodology is tested against the laboratory data from the own measurements as well as the published data in the literature. Over 30 samples are used covering a wide range of the soil textural composition. Final conclusions end the paper.

2. Basic principles and methods of micromechanics

The methods of overall material constants evaluation in terms of constituent properties can be classified into two, methodologically different, approaches: the computational and the analytical micromechanics (e.g. Dormieux and Ulm, 2005; Dormieux et al., 2006). The latter one is classically used if the statistical information on the microstructure is incomplete. Typically, the primary information is available on volume fractions of individual constituents. Furthermore, if there is no preferred arrangement of constituents, i.e. the structure is perfectly disordered, the other statistical information available is that stipulating the isotropy of the medium at the macroscale. In addition, some other information like matrix-inclusion or polycrystalline morphology, the type and the shape of inclusions can be implemented into considerations.

The oldest micromechanical models which take into account only the volume fractions of composite phases are those due to Voigt and Reuss (or Wiener upper and lower bounds) (Milton, 2002; Torquato, 2002). For composite medium comprising M homogeneous constituents with different conductivity properties, they can be presented as

$$\frac{1}{\sum_{i=1}^{M}\frac{c^\alpha}{\lambda^\alpha}} \le \lambda^{hom} \le \sum_{i=1}^{M} c^\alpha \lambda^\alpha \tag{1}$$

where c^α and λ^α are the volume fraction and thermal conductivity coefficient of α-component, respectively.

For a macroscopically isotropic medium, Hashin and Shtrikman (1963) proposed narrower bounds as

$$\frac{1}{\sum_{\alpha=1}^{M}\frac{c^\alpha}{2\lambda_{min}+\lambda^\alpha}} - 2\lambda_{min} \le \lambda^{hom} \le \frac{1}{\sum_{\alpha=1}^{M}\frac{c^\alpha}{2\lambda_{max}+\lambda^\alpha}} - 2\lambda_{max} \tag{2}$$

where

$$\lambda_{min} = \min_\alpha \lambda^\alpha,\ \lambda_{max} = \max_\alpha \lambda^\alpha \tag{3}$$

Beyond the above bounds, the approximate homogenization schemes have been proposed. Among others, the most often used are the Mori–Tanaka and the self-consistent schemes (Mura, 1987; Šejnoha and Zeman, 2002; Li and Wang, 2008). The first one is suitable for composites with matrix-inclusion morphology. No a